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Symplectic Properties of Multistep Runge-Kutta Methods

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Abstract—We investigate the symplecticity of multistep Runge-Kutta methods (MRKMs) as general linear methods (GLMs) for Hamiltonian systems in accordance with the definition due to Bochev and Scovel [1], Eirola and Sanz-Serna [2], and Hairer and Leone [3,4]. We present a necessary and sufficient condition for an MRKM to be symplectic, and show that many typical high-order MRKMs cannot be symplectic unless they degenerate into one-step Runge-Kutta methods (RKMs). We also show that the order of any symplectic two-step RKM is at most 2. We conjecture that there exist order barriers for symplectic MRKMs, and more generally, for symplectic GLMs.

Keywords—Hamiltonian system, Multistep Runge-Kutta method, Symplecticity.

1. INTRODUCTION

Consider the Hamiltonian system with Hamiltonian $H(p,q)$ on R^{2N}

$$\begin{aligned} \frac{dp}{dt} &= -\frac{\partial H}{\partial q}, \\ \frac{dq}{dt} &= \frac{\partial H}{\partial p}, \end{aligned} \tag{1.1}$$

where

$$p = (p_1, p_2, \dots, p_N)^\top, \qquad q = (q_1, q_2, \dots, q_N)^\top.$$

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or equivalently,

$$\frac{dy}{dt} = J\frac{\partial H}{\partial y} := f(y), \tag{1.2}$$

with $y = (p_1, p_2, \ldots, p_N; q_1, q_2, \ldots, q_N)^\top$, $J = \begin{pmatrix} 0 & -I_N \\ I_N & 0 \end{pmatrix}$, here and hereafter, I_l denotes the $l \times l$ identity matrix, $e_l = (1, 1, \ldots, 1)^\top \in R^l$, $l = 1, 2, \ldots$. The phase space R^{2N} is equipped with a standard symplectic structure defined by the fundamental differential 2-form

$$\omega = \frac{1}{2} J^{-1}\, dy \wedge dy = dp \wedge dq = \sum_{i=1}^{N} dp_i \wedge dq_i,$$

where the symbol $\wedge$ denotes exterior product.

In order to solve (1.2), we consider the r-value s-stage GLM (cf. [5,6])

$$\begin{aligned} Y_i^{(n)} &= h\sum_{j=1}^{s} c_{ij}^{11} f\left(Y_j^{(n)}\right) + \sum_{j=1}^{r} c_{ij}^{12} y_j^{(n-1)}, \qquad i = 1, 2, \ldots, s, \\ y_i^{(n)} &= h\sum_{j=1}^{s} c_{ij}^{21} f\left(Y_j^{(n)}\right) + \sum_{j=1}^{r} c_{ij}^{22} y_j^{(n-1)}, \qquad i = 1, 2, \ldots, r, \end{aligned} \tag{1.3}$$

where $h > 0$ is the given step-size, c_{ij}^{IJ} are real constants for any i, j, I, J. The vector $Y_i^{(n)}$ is an internal stage of the current step and is an approximation to $y(t_n + c_i h)$ for $i = 1, 2, \ldots, s$. And, the external stage vectors $y_i^{(n)} = ({p_i^{(n)}}^\top, {q_i^{(n)}}^\top)^\top$, $i = 1, 2, \ldots, r$, contain all information from the previous steps necessary for the computation of the new approximation. Here $t_n = nh$, c_i, and ν_i are real constants. Let

$$\begin{aligned} y^{(n)} &= \left({y_1^{(n)}}^\top, {y_2^{(n)}}^\top, \ldots, {y_r^{(n)}}^\top\right)^\top \in R^{2Nr}, \\ Y^{(n)} &= \left({Y_1^{(n)}}^\top, {Y_2^{(n)}}^\top, \ldots, {Y_s^{(n)}}^\top\right)^\top \in R^{2Ns}, \\ F\left(Y^{(n)}\right) &= h\left(f\left(Y_1^{(n)}\right)^\top, f\left(Y_2^{(n)}\right)^\top, \ldots, f\left(Y_s^{(n)}\right)^\top\right)^\top \in R^{2Ns}, \\ C_{IJ} &= \left[c_{ij}^{IJ}\right], \quad \tilde{C}_{IJ} = C_{IJ} \otimes I_{2N}, \qquad I, J = 1, 2, \end{aligned}$$

where the symbol $A \otimes B$ denotes Kronecker product of the matrices A and B. Then method (1.3) can be written in more compact form

$$\begin{aligned} Y^{(n)} &= \tilde{C}_{11} F\left(Y^{(n)}\right) + \tilde{C}_{12} y^{(n-1)}, \\ y^{(n)} &= \tilde{C}_{21} F\left(Y^{(n)}\right) + \tilde{C}_{22} y^{(n-1)}. \end{aligned} \tag{1.4}$$

It is not trivial to give a natural definition of symplecticity for linear multistep methods, and more generally for general linear methods [5,6]. At present, as pointed out by Hairer and Leone [3–5], there exist two different approaches of the symplecticity of GLMs. But for one-step methods, they are in line. The first approach is to define a GLM to be symplectic if its underlying one-step (or its step-transition operator) is symplectic (cf. [7,8]). Tang [8] proved that consistent linear multistep methods cannot be symplectic. Hairer and Leone [3–5] proved that the order of a GLM has to be at least twice its stage order and gave a conjecture: GLMs which are not one-step methods cannot be symplectic. As a special case, they showed that the implicit midpoint rule is the only irreducible symplectic one-leg method.

The second approach is to extend the differential form $dp \wedge dq$ on R^{2N} to the space $(R^{2N})^r$. Eirola and Sanz-Serna [2] showed that the quadratic invariants and symplecticity of the original systems can be extended to a one-leg method by using a tensor product, and proved that a symmetric irreducible one-leg method preserves the quadratic first integrals and the differential form

$$\sum_{i,j=1}^{r} g_{ij} dp_{n+i} \wedge dq_{n+j},$$

for the symmetric invertible matrix $G = [g_{ij}] \in R^{r\times r}$ (i.e., Λ in [2]) determined by the given one-leg methods. Bochev and Scovel [1] proved that for one-step methods the preservation of the quadratic first integrals is equivalent to the preservation of the symplectic structure when the methods are applied to Hamiltonian systems, and showed that if a GLM preserves the quadratic first integral generated by the quadratic first integral of the original problem, then the method is symplectic with regard to a new symplectic structure in the higher-dimensional space.

DEFINITION 1.1. *(See [1–4].) A GLM is symplectic if there exists an invertible symmetric matrix G such that*

$$y^{(n)^{\top}}(G\otimes S)y^{(n)} = y^{(n-1)^{\top}}(G\otimes S)y^{(n-1)}, \tag{1.5}$$

when applied to a problem which possesses $y^{\top}Sy$ as a quadratic first integral.

THEOREM 1.2. *(See [3–5,9].) Assume that there exist an invertible real symmetric $r\times r$ matrix $G=[g_{ij}]$ and a nonzero real diagonal $s\times s$ matrix $D=\operatorname{diag}(d_1,d_2,\dots,d_s)$ such that the matrix*

$$M = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22}\end{pmatrix} = 0, \tag{1.6}$$

where

$$\begin{gathered} M_{11} = G - C_{22}^{\top}GC_{22}, \qquad M_{12} = M_{21}^{\top} = C_{12}^{\top}D - C_{22}^{\top}GC_{21}, \\ M_{22} = C_{11}^{\top}D + DC_{11} - C_{21}^{\top}GC_{21}. \end{gathered}$$

Then method (1.3) applied to system (1.2) is symplectic under Definition 1.1.

CONJECTURE 1.3. *(See [3,4].) For irreducible GLMs, the condition $M=0$ is also necessary for symplecticity.*

Hereafter, the expression "a GLM is symplectic" means "$M=0$". Hairer and Leone [5] and Xiao *et al.* [9] showed that $M=0$ implies

$$\sum_{i,j=1}^{r} g_{ij} dp_i^{(n)} \wedge dq_j^{(n)} = \sum_{i,j=1}^{r} g_{ij} dp_i^{(n-1)} \wedge dq_j^{(n-1)}. \tag{1.7}$$

Xiao *et al.* also showed that irreducible symmetric one-leg methods written in the form of the GLM (1.4) as in [1] satisfy (1.6) for the matrix G (i.e., Λ in [2]). This result together with the results given in [2] proves Conjecture 1.3 for one-leg methods. It is well known that Theorem 1.2 and Conjecture 1.3 hold for irreducible RKMs written in the form of the GLM (1.4) as in [10] (for example, cf. [11]). Unfortunately, BDF methods are not symplectic for lack of symmetry. In [9], it is also shown that linear two-step second-order methods written in the form of the GLM (1.4) as in [10] cannot be symplectic. Moreover, it easily follows from the equality $M_{11}=0$ in the symplectic condition (1.6) that the GLM (1.4) with $r\ge 2$ and $\operatorname{rank}(C_{22})=1$ (such as DIMSIMs in [12]) cannot be symplectic.

In the sequel, we investigate the symplectic properties of MRKMs, regarded as GLMs for Hamiltonian systems according to the above definition of symplecticity. In Section 2, we present a necessary and sufficient condition for a MRKM to be symplectic, and show that many typical high-order MRKMs cannot be symplectic (with regard to the symmetric invertible matrix G with $\sum_{j=1}^{r} g_{rj} = g_{rr}$) unless they degenerate into one-step RKMs. In Section 3, we show that the order of a symplectic two-step RKM is at most 2. We conjecture that there exist order barriers for symplectic MRKMs, and more generally, for symplectic GLMs. Furthermore, the above facts lead to such an open problem: can we find high-order symplectic MRKMs (or in general, symplectic GLMs)?

2. SYMPLECTIC PROPERTIES OF MRKMS

When a MRKM applied to (1.2)

$$\begin{aligned} Y_i^{(n)} &= h\sum_{j=1}^{s} b_{ij} f\left(Y_j^{(n)}\right) + \sum_{j=1}^{r} a_{ij} y_{j+n-1}, \qquad i = 1,2,\dots,s, \\ y_{n+r} &= h\sum_{j=1}^{s} \gamma_j f\left(Y_j^{(n)}\right) + \sum_{j=1}^{r} \alpha_j y_{j+n-1}, \end{aligned} \tag{2.1}$$

is written as a general linear method (1.3) (cf. [13–15]), we have

$$y_j^{(n-1)} = y_{j+n-1}, \qquad y_r^{(n)} = y_{n+r},$$

$$C_{11} = B = [b_{ij}] \in R^{s\times s}, \qquad C_{12} = A = [a_{ij}] \in R^{s\times r},$$

$$C_{21} = \begin{pmatrix} 0 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & 0 \\ \gamma_1 & \gamma_2 & \dots & \gamma_s \end{pmatrix} \in R^{r\times s}, \qquad C_{22} = \begin{pmatrix} 0 & 1 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & 1 \\ \alpha_1 & \alpha_2 & \dots & \alpha_r \end{pmatrix} \in R^{r\times r},$$

where $b_{ij}, a_{ij}, \gamma_i, \alpha_i$ are real constants. Let us set

$$\gamma = (\gamma_1, \gamma_2, \dots, \gamma_s)^\top \in R^s, \qquad \alpha = (\alpha_1, \alpha_2, \dots, \alpha_r)^\top \in R^r.$$

And, we always assume that

$$\sum_{j=1}^{r} \alpha_j = 1, \quad \sum_{j=1}^{r} a_{ij} = 1, \qquad i = 1,2,\dots,s, \tag{2.2a}$$

$$c_i \neq c_j, \quad \text{for } i \neq j, \qquad \gamma_i \neq 0, \qquad i,j = 1,2,\dots,s, \tag{2.2b}$$

where relation (2.2a) is said to be *"the preconsistency condition"*. For the family of MRKMs given by (2.1) one can easily show

$$(M_{11})_{ij} = g_{ij} - g_{rr}\alpha_i\alpha_j - g_{r,j-1}\alpha_i - g_{i-1,r}\alpha_j - g_{i-1,j-1}, \qquad i,j = 1,2,\dots,r, \tag{2.3}$$

$$(M_{21})_{ij} = (M_{12})_{ji} = -g_{rr}\gamma_i\alpha_j - g_{r,j-1}\gamma_i + a_{ij}d_i, \qquad j = 1,2,\dots,r, \quad i = 1,2,\dots,s, \tag{2.4}$$

$$(M_{22})_{ij} = -g_{rr}\gamma_i\gamma_j + d_i b_{ij} + d_j b_{ji}, \qquad i,j = 1,2,\dots,s, \tag{2.5}$$

where $g_{i0} = g_{0i} = 0$, $i = 0,1,2,\dots,r$. It follows from (2.3)–(2.5), Theorem 5.3 in [10] and the facts $\det G \neq 0$, $\gamma_i \neq 0$, $i = 1,2,\dots,s$, that $M = 0$ iff

$$\begin{gathered} g_{rr} = 2\kappa\lambda, \qquad g_{r,j-1} = \kappa(a_j - 2\lambda\alpha_j), \quad j = 2,3,\dots,r, \\ g_{ij} = g_{i-1,j-1} + \kappa(a_j\alpha_i + \alpha_j a_i - 2\lambda\alpha_i\alpha_j), \qquad i,j = 1,2,\dots,r, \\ \kappa = \sum_{j=1}^{r} g_{rj} \neq 0, \end{gathered} \tag{2.6}$$

$$d_i = \kappa\gamma_i, \qquad i = 1,2,\dots,s, \tag{2.7}$$

$$
\begin{gathered}
a_j := a_{kj} = a_{lj}, \qquad k \neq l, k, l = 1, 2, \dots, s, \quad j = 1, 2, \dots, r, \\
b_{ii} = \lambda \gamma_i, \qquad i = 1, 2, \dots, s, \\
a_1 = 2\lambda\alpha_1, \qquad a_2 = 2\lambda\alpha_2 + \alpha_1 a_r, \\
\gamma_i b_{ij} + \gamma_j b_{ji} - 2\lambda\gamma_i\gamma_j = 0, \qquad i, j = 1, 2, \dots, s,
\end{gathered} \tag{2.8}
$$

where $\lambda \in R$ is a parameter. Moreover, it follows from the second formula in (2.6) that

$$
\begin{aligned}
g_{ii} &= 2\kappa \left(\lambda - \sum_{m=i+1}^{r} \left(\alpha_m a_m - \lambda \alpha_m^2 \right) \right), \\
g_{r-l,j-l} &= \kappa(a_{j+1} - 2\lambda\alpha_{j+1} - \sigma(j,l)), \\
\sigma(j,l) &= \sum_{m=0}^{l-1} (\alpha_{r-m} a_{j-m} + \alpha_{j-m} a_{r-m} - 2\lambda \alpha_{r-m} \alpha_{j-m}),
\end{aligned} \tag{2.9}
$$

where $i = 1, 2, \dots, r-1$, $j = 2, 3, \dots, r-1$, $l = 1, 2, \dots, j-1$. From Theorem 1.2, Conjecture 1.3, and the above deduction, we have the following.

THEOREM 2.1. *If the matrix G given by (2.6) and (2.9) is nonsingular, i.e., $\det G \neq 0$, then method (2.1) satisfying (2.8) is symplectic (under Definition 1.1) for system (1.2).*

REMARK 2.2. Conditions (2.8) imply the matrix $A = e_s a^\top$ with $a^\top = (a_1, a_2, \dots, a_r)$. Generally, it is difficult to determine whether the above matrix G is singular. Now in order to obtain some results, we combine the condition $M = 0$ with the order conditions of method (2.1).

Let us introduce the following simplifying conditions (cf. [13–15])

$$
\begin{aligned}
&B(\eta) : \alpha^\top \chi^k = r^k - k\gamma^\top c^{k-1}, && k = 1, 2, \dots, \eta, \\
&C(\eta) : A\chi^k = c^k - kBc^{k-1}, && k = 1, 2, \dots, \eta, \\
&D(\eta) : k\gamma^\top C^{k-1} B = r^k \gamma^\top - \gamma^\top C^k, && k = 1, 2, \dots, \eta, \\
&E(\eta) : kA^\top \operatorname{diag}(\gamma) c^{k-1} = \operatorname{diag}(\alpha) \left(r^k e_r - \chi^k \right), && k = 1, 2, \dots, \eta,
\end{aligned}
$$

where $C = \operatorname{diag}(c)$, $c = (c_1, c_2, \dots, c_s)^\top$, $\chi = (0, 1, \dots, r-1)^\top$, and multiplication of vectors is done componentwise.

We congruently transform M into

$$
\hat{M} = X^\top M X = \begin{pmatrix} M_{11} & M_{21}^\top V \\ V^\top M_{21} & V^\top M_{22} V \end{pmatrix}, \qquad X = \begin{pmatrix} I_r & 0 \\ 0 & V \end{pmatrix},
$$

where $V = [\delta_{j-1}(c_i)]$ is an $s \times s$ generalized Vandermonde matrix, and $\delta_{j-1}(x)$ is arbitrary polynomial of degree $j-1$ ($j = 1, 2, \dots$). Let $\tilde{R} = [r_{lm}] = V^\top M_{22} V$. It follows from (2.5) and (2.7) that the (l,m)-element of $\tilde{R}$ is

$$
\begin{aligned}
r_{lm} = \kappa &\left(\sum_{i,j=1}^{s} \left(\gamma_i \delta_{l-1}(c_i) b_{ij} \delta_{m-1}(c_j) + \gamma_i \delta_{m-1}(c_i) b_{ij} \delta_{l-1}(c_j) \right) \right) \\
&- g_{rr} \sum_{i=1}^{s} \gamma_i \delta_{l-1}(c_i) \sum_{j=1}^{s} \gamma_j \delta_{m-1}(c_j), \qquad l, m = 1, 2, \dots, s.
\end{aligned} \tag{2.10}
$$

If we choose $\delta_0(x), \delta_1(x), \dots, \delta_{s-1}(x)$ such that

$$
\delta_j(x) = \rho_{j+1}'(x), \qquad j = 0, 1, \dots, s-1, \tag{2.11}
$$

where $\rho_{j+1}(x) = \prod_{k=0}^{j}(x-k)$, then the conditions $B(\eta)$, $C(\eta)$, $D(\eta)$, and $E(\eta)$ are equivalent to

$$\sum_{i=1}^{s}\gamma_i\rho_l'(c_i)=\rho_l(r)-\sum_{j=1}^{r}\alpha_j\rho_l(j-1),\qquad l=1,2,\dots,\eta, \tag{2.12}$$

$$\sum_{j=1}^{s}b_{ij}\rho_l'(c_j)=\rho_l(c_i)-\sum_{j=1}^{r}a_{ij}\rho_l(j-1),\qquad l=1,2,\dots,\eta,\quad i=1,2,\dots,s, \tag{2.13}$$

$$\sum_{i=1}^{s}\gamma_i\rho_l'(c_i)b_{ij}=\gamma_j(\rho_l(r)-\rho_l(c_j)),\qquad l=1,2,\dots,\eta,\quad j=1,2,\dots,s, \tag{2.14}$$

$$\sum_{i=1}^{s}\gamma_i\rho_l'(c_i)a_{ij}=\alpha_j(\rho_l(r)-\rho_l(j-1)),\qquad l=1,2,\dots,\eta,\quad j=1,2,\dots,r, \tag{2.15}$$

respectively. In fact, let $\delta_{j-1}(x)=\sum_{i=0}^{j-1}\phi_i x^i$. Then, it follows from (2.11) that $\rho_j(x)=\sum_{i=1}^{j}\phi_{i-1}x^i/i$. $B(\eta)$ implies

$$\sum_{i=1}^{s}\gamma_i c_i^{k-1}=\frac{r^k}{k}-\sum_{i=1}^{r}\alpha_i\,\frac{(i-1)^k}{k},\qquad k=1,2,\dots,\eta.$$

Multiplying the two sides of the above formula by ϕ_{k-1} and adding up for $k=1,2,\dots,l$ yield (2.12), where $l=1,2,\dots,\eta$. On the other hand, assume that (2.12) holds. We can take $\delta_{k-1}(x)=kx^{k-1}$ for $k=1,2,\dots,\eta$. Hence, $\rho_k(x)=x^k$, $k=1,2,\dots,\eta$. $B(\eta)$ follows from substituting the formulas $\rho_k(x)=x^k$ ($k=1,2,\dots,\eta$) into (2.12). Similarly, we can prove that the conditions $C(\eta)$, $D(\eta)$, and $E(\eta)$ are equivalent to (2.13), (2.14), and (2.15), respectively.

LEMMA 2.3. *If the MRKM (2.1) is symplectic under Definition 1.1, but with $\kappa=g_{rr}$ and satisfies $q\ge r-1$, $B(\max\{r,q\})$ and one of the following two conditions:*

(1) *$D(q)$;*
(2) *$C(q)$ and $E(q)$,*

then $B(2q)$ holds and

$$\alpha_i^2=\alpha_i,\qquad \alpha_i\alpha_j=0\quad(i\ne j),\qquad i,j=1,2,\dots,r. \tag{2.16}$$

PROOF. First, let us assume that $D(q)$ holds. It follows from (2.14) that

$$\sum_{i,j=1}^{s}\gamma_i\rho_l'(c_i)b_{ij}\rho_m'(c_j)=\sum_{j=1}^{s}\gamma_j\rho_m'(c_j)(\rho_l(r)-\rho_l(c_j)),\qquad l,m=1,2,\dots,q. \tag{2.17}$$

Upon substituting $B(q)$, (2.17) and (2.11) into (2.10) we obtain

$$\begin{aligned} r_{lm}=-B_{lm}&+(\kappa-g_{rr})\left(\rho_l(r)-\sum_{j=1}^{r}\alpha_j\rho_l(j-1)\right)\left(\rho_m(r)-\sum_{j=1}^{r}\alpha_j\rho_m(j-1)\right)\\ &+\kappa\left(\sum_{j=1}^{r}\alpha_j\rho_l(j-1)\rho_m(j-1)-\sum_{j=1}^{r}\alpha_j\rho_l(j-1)\sum_{j=1}^{r}\alpha_j\rho_m(j-1)\right), \end{aligned} \tag{2.18}$$

where $l,m=1,2,\dots,q$. And

$$B_{lm}=\kappa\left(\sum_{j=1}^{r}\alpha_j\rho_l(j-1)\rho_m(j-1)+\sum_{i=1}^{s}\gamma_i(\rho_l(c_i)\rho_m(c_i))'-\rho_l(r)\rho_m(r)\right).$$

Since $\kappa=g_{rr}$ and $\rho_l(j)=0$ for $j=0,1,\dots,l-1$, it follows from (2.18) that

$$r_{lm}=-B_{lm},\qquad \text{for } l,m=1,2,\dots,q,\quad l>r-1 \text{ or } m>r-1. \tag{2.19a}$$

Thus, (2.19a), $B(\max\{r,q\})$, and the symplecticity of the methods yield that $B(2q)$ holds. And, it follows from $B(2q)$ and the inequality $q > r-1$ that $B(2r-2)$ holds and

$$r_{lm} = \kappa\left(\sum_{j=1}^{r}\alpha_j\rho_l(j-1)\rho_m(j-1) - \sum_{j=1}^{r}\alpha_j\rho_l(j-1)\sum_{j=1}^{r}\alpha_j\rho_m(j-1)\right), \tag{2.19b}$$

for $l,m = 1,2,\dots,r-1$. Moreover, (2.19b) and the symplecticity of the methods yield

$$\sum_{j=1}^{r}\alpha_j\rho_l(j-1)\rho_m(j-1) = \sum_{j=1}^{r}\alpha_j\rho_l(j-1)\sum_{j=1}^{r}\alpha_j\rho_m(j-1), \qquad l,m = 1,2,\dots,r-1. \tag{2.20}$$

Let $\hat{R} = [r_{lm}] \in R^{(r-1)\times(r-1)}$. Then (2.19b) and (2.20) yield

$$\hat{R} = \kappa U^\top \bar{R} U = 0, \tag{2.21}$$

where $U = [\rho_j(i)] \in R^{(r-1)\times(r-1)}$, and

$$\bar{R} = \operatorname{diag}(\alpha_2,\alpha_3,\dots,\alpha_r) - \hat{\alpha}\hat{\alpha}^\top, \qquad \hat{\alpha}^\top = (\alpha_2,\alpha_3,\dots,\alpha_r).$$

$\hat{R} = 0$ means $\bar{R} = 0$, i.e.,

$$\alpha_i^2 = \alpha_i, \qquad \alpha_i\alpha_j = 0 \quad (i \neq j), \qquad i,j = 2,\dots,r.$$

Moreover, (2.16) holds because $\alpha^\top e_r = 1$.

The proof of case (2) is similar to that of case (1). ∎

LEMMA 2.4. *If method (2.1) is symplectic and satisfies $B(q)$, $E(q)$, and (2.16), then $g_{r,m-1} = 0$, $m = 1,2,\dots,r$.*

PROOF. The symplecticity of (2.1) means that $V^\top M_{21} = 0$, i.e.,

$$\kappa\sum_{i=1}^{s}\gamma_i\rho_l'(c_i)(a_{im} - \alpha_m) - g_{r,m-1}\sum_{i=1}^{s}\gamma_i\rho_l'(c_i) = 0, \tag{2.22}$$

for $l = 1,2,\dots,s$, $m = 1,2,\dots,r$. $B(q)$, $E(q)$, and (2.22) yield

$$\kappa\alpha_m\left(\sum_{j=1}^{r}\alpha_j\rho_l(j-1) - \rho_l(m-1)\right) + g_{r,m-1}\left(\sum_{j=1}^{r}\alpha_j\rho_l(j-1) - \rho_l(r)\right) = 0, \tag{2.23}$$

for $l = 1,2,\dots,q$, $m = 1,2,\dots,r$. Moreover, (2.16) leads to

$$\kappa\alpha_m\left(\sum_{j=1}^{r}\alpha_j\rho_l(j-1) - \rho_l(m-1)\right) = 0.$$

Thus, (2.23) yields

$$\Delta_{lm} := g_{r,m-1}\left(\sum_{j=1}^{r}\alpha_j\rho_l(j-1) - \rho_l(r)\right) = 0, \qquad l = 1,2,\dots,q, \quad m = 1,2,\dots,r. \tag{2.24}$$

When $q \geq r$, $\Delta_{rm} = -g_{r,m-1}\rho_r(r) = 0$, hence, $g_{r,m-1} = 0$ for $m = 1,2,\dots,r$.

When $q = r-1$, (2.16) means that there exists j_0 $(1 \leq j_0 \leq r)$ such that $\alpha_{j_0} = 1$, $\alpha_j = 0$ $(j \neq j_0)$, and

$$\Delta_{r-1,m} = g_{r,m-1}(\rho_{r-1}(j_0 - 1) - \rho_{r-1}(r)) = 0,$$

moreover, for $m = 1,2,\dots,r$,

$$\Delta_{r-1,m} = \begin{cases} -g_{r,m-1}\rho_{r-1}(r) = 0, & j_0 \leq r-1, \\ g_{r,m-1}((r-1)! - r!) = 0, & j_0 = r. \end{cases}$$

Therefore, $g_{r,m-1} = 0$ for $m = 1,2,\dots,r$. ∎

THEOREM 2.5. *The nondegenerate method (2.1) satisfying $B(\max\{r,q\})$, $q \geq r-1$, $C(q)$, (or $D(q)$) and $E(q)$ cannot be symplectic under Definition 1.1 with $\kappa = g_{rr}$.*

PROOF. Theorem 2.5 can be easily obtained from Lemma 2.3, Lemma 2.4, and the equalities (2.6)–(2.9). In fact, it follows from (2.16) that there exists i_0 ($1 \leq i_0 \leq r$) such that $\alpha_{i_0} = 1$, $\alpha_i = 0$ ($i \neq i_0$), $i = 1,2,\dots,r$. Moreover, together with the equalities $\kappa = g_{rr}$ and $g_{r,m-1} = 0$ ($m = 1,2,\dots,r$), (2.16) yields $2\lambda = 1$, $a = \alpha$, and

$$g_{ij} = \begin{cases} \kappa, & \text{for } i = j,\ i \geq i_0, \\ 0, & \text{for } i \neq j \text{ or } i = j,\ i < i_0. \end{cases}$$

Thus, G is diagonal. In this case, method (2.1) degenerates into the one-step RK method with step-size $(r - i_0 + 1)h$

$$\begin{array}{c|c} c & \dfrac{B}{(r-i_0+1)} \\ \hline & \dfrac{\gamma^\top}{(r-i_0+1)} \end{array} \tag{2.25}$$ ∎

REMARK 2.6. For method (2.1) satisfying the conditions assumed in Theorem 2.5, it follows from the proof of Theorem 2.5 that (1.5) becomes

$$\sum_{i=i_0}^{r} y_i^{(n)\top} S y_i^{(n)} = \sum_{i=i_0}^{r} y_i^{(n-1)\top} S y_i^{(n-1)},$$

i.e.,

$$y_r^{(n)\top} S y_r^{(n)} = y_{i_0}^{(n-1)\top} S y_{i_0}^{(n-1)} \quad \text{or} \quad y_{n+r}^\top S y_{n+r} = y_{n+i_0-1}^\top S y_{n+i_0-1}. \tag{2.26}$$

In the same way, (1.7) becomes

$$dp_{n-1+i_0} \wedge dq_{n-1+i_0} = dp_{n+r} \wedge dp_{n+r}. \tag{2.27}$$

Equations (2.26) and (2.27) imply that method (2.25) is symplectic and preserves the quadratic invariant $y^\top Sy$.

REMARK 2.7. Li [15] presented six classes of high-order MRKMs which include the class given by Burrage [13]. These six classes of MRKMs include

Class 1 : $B(2s), E(s), C(s)$(or $D(s)$);
Class 2 : $B(2s-1), E(s), C(s)$ with some conditions;
Class 3 : $B(2s-1), E(s), D(s)$ with some conditions;
Class 4 : $B(\max\{2s-2,s\}), E(s), C(s-1)$ with some conditions;
Class 5 : $B(\max\{2s-3,s\}), E(s), C(s-1)$ with some conditions;
Class 6 : $B(\max\{2s-3,s\}), E(s), D(s-1)$ with some conditions.

The contents of "some conditions" have been given in [15]. We do not need them here. From Theorem 2.5, we easily show that Li's Class 1 with the inequalities $2s \geq r$ and $s \geq r-1$, Li's Classes 2 and 3 with $2s \geq r+1$ and $s \geq r-1$ and Li's Classes 4–6 with $s \geq r$ in [15] cannot be symplectic (for the matrix G given by (2.6), (2.9), and with $\kappa = g_{rr}$). Hence, a possible approach by which high-order symplectic MRKMs ($r \geq 3$) can be constructed is to consider G with $\kappa \neq g_{rr}$.

3. SYMPLECTIC PROPERTIES OF TWO-STEP RKMS

In this section, we investigate the symplectic properties of two-step RKMs (i.e., MRKMs (2.1) with $r = 2$). It follows from (2.6)–(2.9) that

$$\begin{gathered} \alpha = (1,0)^{\mathsf{T}}, \qquad a^{\mathsf{T}} = (2\lambda, 1-2\lambda)^{\mathsf{T}}, \qquad g_{ii} = 2\kappa\lambda, \\ g_{ij} = \kappa(1-2\lambda), \qquad i \neq j, \quad i,j = 1,2, \end{gathered} \tag{3.1}$$

$$\tilde{M}_{22} := [\gamma_i b_{ij} + \gamma_j b_{ji} - 2\lambda\gamma_i\gamma_j] \in R^{s\times s} = 0, \qquad b_{ii} = \lambda\gamma_i, \quad i = 1,2,\dots,s, \tag{3.2}$$

where $\lambda \in R$ is one parameter. When $2\lambda = 1$, these methods degenerate into one-step RKMs with the step-size $2h$

$$\begin{array}{c|c} c & \dfrac{B}{2} \\ \hline & \dfrac{\gamma^{\mathsf{T}}}{2} \end{array}.$$

And in this case, $\kappa = g_{rr}$, and the conclusion of Theorem 2.5 naturally holds. Therefore, the symplecticity of two-step RKMs need further study. In fact, we have found that there is also an order barrier for symplectic two-step Runge-Kutta methods.

THEOREM 3.1. *The order of symplectic nondegenerate two-step RKMs satisfying $C(1)$ is at most 2.*

PROOF. If symplectic two-step RKMs satisfying $C(1)$ are of order 3, then it follows from Theorem 2.2 in [13] that $B(3)$ holds and

$$\gamma^{\mathsf{T}} c^2 - \gamma^{\mathsf{T}} A\chi^2 - 2\gamma^{\mathsf{T}} Bc = 0. \tag{3.3}$$

These yield

$$\gamma^{\mathsf{T}} Bc = 2\lambda + \frac{1}{3}. \tag{3.4}$$

On the other hand, it follows from $e_s^{\mathsf{T}} \tilde{M}_{22} c = 0$ that

$$\gamma^{\mathsf{T}} Bc = 4\lambda - \frac{2}{3}. \tag{3.5}$$

Equations (3.4) and (3.5) lead to $2\lambda = 1$. ∎

From (3.1) and (3.2), we easily obtain the following.

THEOREM 3.2.

(1) *Symplectic nondegenerate two-step RKMs do not satisfy $E(1)$.*
(2) *Symplectic nondegenerate two-step RKMs satisfying $C(1)$ and $B(2)$ do not imply $D(1)$.*

COROLLARY 3.3. *All nondegenerate two-step RKMs of order≥ 3 cannot be symplectic (with regard to the invertible matrix G given by (3.1)). All nondegenerate two-step RKMs satisfying $E(1)$ or $B(2)$, $C(1)$, and $D(1)$ cannot be symplectic.*

Corollary 3.3 shows that the six classes of two-step high-order RKMs presented in [15] cannot be symplectic unless they are degenerate. These facts together with Theorem 2.5 and Remark 2.7 lead to the following conjecture.

CONJECTURE 3.4. *There exist order barriers of symplectic MRKMs, and more generally, for symplectic GLMs.*

Now we give an example of symplectic two-step RKMs. By Theorem 3.1, we need only to consider second-order methods. The class of symplectic two-step two-stage second-order RKMs with stage order 2 is constructed as follows:

$$\alpha = (1,0)^\top \qquad \gamma^\top = (1,1), \qquad 2\lambda = 3(1-c_1)^2, \qquad c_2 = 2 - c_1,$$

$$A = \begin{pmatrix} 3(1-c_1)^2 & 1-3(1-c_1)^2 \\ 3(1-c_1)^2 & 1-3(1-c_1)^2 \end{pmatrix}, \qquad B = \begin{pmatrix} 3(1-c_1)^2/2 & (c_1-1)(3c_1-1)/2 \\ (1-c_1)(5-3c_1)/2 & 3(1-c_1)^2/2 \end{pmatrix},$$

where c_1 is one parameter, $c_1 \neq 1$ (because of $c_1 \neq c_2$), and $c_1 \neq (3\pm\sqrt{3})/3$ (because of $2\lambda \neq 1$). This given class of symplectic two-step RKMs is also symmetric under the symmetry definition of GLMs in [4].

4. CONCLUSIONS AND FURTHER WORK

We have studied some symplectic properties of MRKMs, regarded as GLMs for Hamiltonian systems according to a kind of definition of symplecticity due to Bochev and Scovel, Eirola and Sanz-Serna, and Hairer and Leone, and given a necessary and sufficient condition for an MRKM to be symplectic. Especially, we have shown that many typical high-order MRKMs cannot be symplectic (with regard to the symmetric invertible matrix G with $\sum_{j=1}^{r} g_{rj} = g_{rr}$) unless they degenerate into one-step RKMs, and that the order of a symplectic two-step RKM is at most 2. These facts lead to an open problem: *can one find high order symplectic MRKMs (or in general, symplectic GLMs)?* It would be an interesting but uneasy job to solve this open problem. A possible approach to construct high-order symplectic MRKMs ($r \geq 3$) is to consider G with $\kappa \neq g_{rr}$. On the other hand however, there might exist order barriers for symplectic MRKMs, and more generally, for symplectic GLMs.

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